Simple model of anisotropic pairing with repulsive interactions.

F. Guinea
Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain.
(Dated: February 1, 2008)

A simple tight binding model with repulsive interactions is studied. The inclusion of more than one orbital per site leads to assisted hopping effects, and, when the orbitals involved have different symmetries, to an anisotropic superconducting phase. Superconductivity exists for all fillings, and for all values of the on site repulsion.

PACS numbers: 71.10.Fd, 71.10.Pm, 74.20.Mn, 74.20.Rp

Introduction. The existence of superconductivity in models of strongly correlated electrons with only repulsive interactions has attracted a great deal of attention in recent times. It was established, after the formulation of the BCS theory, that the metallic state is unstable towards anisotropic superconductivity, due to the angular dependence of the dielectric constant[1]. This Kohn-Luttinger instability is greatly enhanced when the Fermi surface in anisotropic[2,3,4]. By using RPA or model dielectric functions, it can also be shown that isotropic Fermi surfaces give rise to anisotropic superconductivity[5]. Varied numerical evidence suggests that models with purely repulsive interactions can lead to anisotropic superconductivity[6,7,8,9].

An alternative scheme which leads to a superconducting ground state starting from models with repulsive interactions was proposed in[10,11]. This model includes an assisted hopping term which arises naturally when considering many orbitals at each lattice site. This assisted hopping term strongly favors the existence of a superconducting ground state[10,11,12]. In its standard version, this model leads to isotropic superconductivity for small hole concentrations, and for a moderate value of the onsite repulsion. In this work, we present an extension of this model which has an anisotropic superconducting ground state for all dopings and arbitrary values of the onsite repulsion.

The model. We study the simplest model with the features discussed above. We postpone to the conclusions the analysis of possible generalizations. Following the scheme in[10], we assume an atom with two orbitals per site on a slightly distorted square lattice. The distortion makes the lattice orthorhombic. We assume that this distortion is small, and we will treat its effects as a perturbation. Using the tetragonal symmetry of the undistorted lattice, we take the lowest lying orbital to be $d_{x^2-y^2}$, and the second orbital to be s or $d_{3z^2-r^2}$. We define $\Delta = \epsilon_s - \epsilon_{x^2-y^2}$ as the difference between the energy of these levels. Without loss of geenrality, we set $\epsilon_d = 0$. We assume that there is only repulsion between electrons in the $d_{x^2-y^2}$ orbital, U. Hopping can take place only between nearest neighbors, with amplitudes t_{ss}, t_{sd} and t_{dd}. Finally, crystal field effects associated to the orthorhombic distortion induce an hybridization between the s and $d_{x^2-y^2}$ in the same site, V_{CF}. The hamiltonian is:

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_{ion} + \mathcal{H}_{tunn} \\
\mathcal{H}_{ion} &= \sum_{\sigma i} \Delta c^\dagger_{s\sigma i} c_{s\sigma i} + U n_{d\uparrow i} n_{d\downarrow i} + \sum_{\sigma i} V_{CF} c^\dagger_{s\sigma i} c_{d\sigma i} + h.c. \\
\mathcal{H}_{tunn} &= \sum_{ij\sigma} t_{dd} c^\dagger_{d\sigma i} c_{d\sigma j} + t_{ss} c^\dagger_{s\sigma i} c_{s\sigma j} \pm t_{sd} c^\dagger_{s\sigma i} c_{d\sigma j} + h.c.
\end{aligned} \tag{1}$$

For simplicity, we neglect here possible differences between the hoppings in the two directions due to the asymmetry of the lattice[13], which is included through the crystal field potential V_{CF} only. Note that, due to the different symmetries of the two orbitals, the hopping between an s and a d orbital has opposite sign along the two axes of the lattice (see fig.[1]).

We now assume that $V_{CF} \ll U, |t_{ss}|, |t_{sd}|, |t_{dd}| \ll \Delta$. The lowest lying eigenstates of $\mathcal{H}_{ion}$ for each occupancy are:

$$\begin{aligned}
|0\rangle &= |0\rangle \\
|1\rangle_\sigma &\approx \left(c^\dagger_{d\sigma} + \frac{V_{CF}}{\Delta} c^\dagger_{s\sigma} \right) |0\rangle \\
|2\rangle &\approx c^\dagger_{d\uparrow} c^\dagger_{d\downarrow} |0\rangle + \frac{V_{CF}}{\Delta - U} \left(c^\dagger_{d\uparrow} c^\dagger_{s\downarrow} + c^\dagger_{s\uparrow} c^\dagger_{d\downarrow} \right) |0\rangle
\end{aligned} \tag{2}$$

with energies:

$$E_0 = 0$$

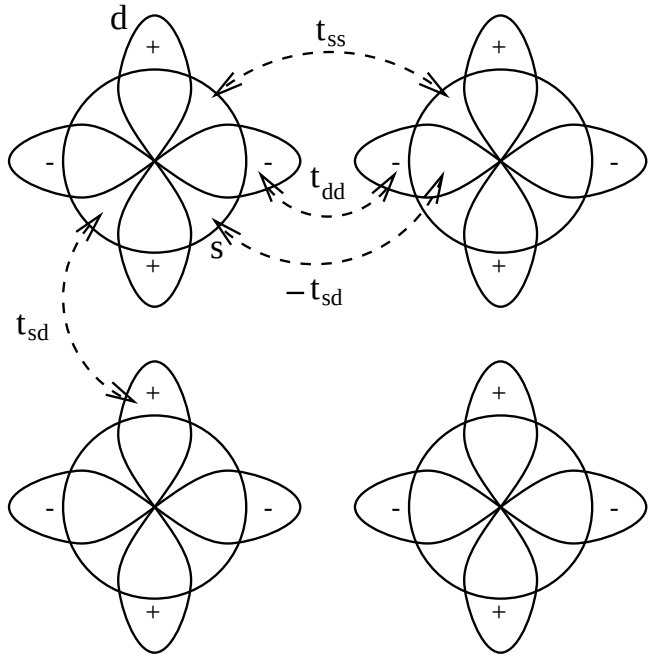

FIG. 1: Sketch of the hopping terms between the two orbitals in the unit cell.

$$\begin{aligned} E_1 &\approx -\frac{V_{CF}^2}{\Delta} \\ E_2 &\approx U - 2\frac{V_{CF}^2}{(\Delta - U)} \end{aligned} \tag{3}$$

Using eq.(2) we define an effective hopping which depends on the occupancy of the site. We find:

$$\begin{aligned} \langle 0_i|\langle 1_{\sigma j}|\mathcal{H}_{tunn}|1_{\sigma i}\rangle|0_j\rangle &\approx t_{dd} \pm 2t_{sd}\frac{V_{CF}}{\Delta} \\ \langle 1_{\uparrow i}|\langle 1_{\downarrow j}|\mathcal{H}_{tunn}|2_i\rangle|0_j\rangle &\approx t_{dd} \pm t_{sd}\left(\frac{V_{CF}}{\Delta} + \frac{V_{CF}}{\Delta - U}\right) \\ \langle 1_{\sigma i}|\langle 2_j|\mathcal{H}_{tunn}||2_i\rangle 1_{\sigma j}\rangle &\approx t_{dd} \pm 2t_{sd}\frac{V_{CF}}{\Delta - U} \end{aligned} \tag{4}$$

We can now write an effective hamiltonian:

$$\mathcal{H}_{eff} = \sum_i \tilde{U}\tilde{n}_{i\uparrow}\tilde{n}_{j\downarrow} + \sum_{\sigma ij} \tilde{t}_{\pm}\tilde{c}^{\dagger}_{\sigma i}\tilde{c}_{\sigma j} \pm \delta t(\tilde{n}_{\sigma i} + \tilde{n}_{\sigma j})\tilde{c}^{\dagger}_{-\sigma i}\tilde{c}_{-\sigma j} + h.c. \tag{5}$$

where we have shifted the origin of energies by $-V_{CF}^2/\Delta$, see eq.(3), and:

$$\begin{aligned} \tilde{c}_{\sigma i} &\approx c_{d\sigma i} + \frac{V_{CF}}{\Delta}c_{s\sigma i} \\ \tilde{t}_{\pm} &\approx t_{dd} \pm 2t_{sd}\frac{V_{CF}}{\Delta} \\ \delta\tilde{t} &\approx 2t_{sd}\frac{V_{CF}U}{\Delta^2} \\ \tilde{U} &\approx U - 2\frac{UV_{CF}^2}{\Delta^2} \end{aligned} \tag{6}$$

Note that, as we are expanding to first order in V_{CF}/Δ, we can neglect normalization terms in the definition of the electron operators $\tilde{c}_{\sigma i}$. For the same reason, $\delta\tilde{t}$ has the same absolute value along the two axes of the lattice. The symmetries of the orbitals involved imply that, to first order, there are not next nearest neighbor assisted hopping terms.

Superconducting solution. The energy bands of the effective hamiltonian, eq.(5), are:

$$\epsilon_{k_x k_y} = \left(\tilde{t}_+ + \frac{n}{2}\delta\tilde{t}\right)\cos(k_x) + \left(\tilde{t}_- - \frac{n}{2}\delta\tilde{t}\right)\cos(k_y) \tag{7}$$

Where n is the number of electrons in the unit cell.

The pairing interaction is[10]:

$$V_{k_x k_y k'_x k'_y} = \tilde{U} + \delta\tilde{t}\left[\cos(k_x) - \cos(k_y) + \cos(k'_x) - \cos(k'_y)\right] \tag{8}$$

The superconducting gap must be of the form:

$$\Delta_{sc\, k_x k_y} = a + b\left[\cos(k_x) - \cos(k_y)\right] \tag{9}$$

Following ref.[10], at the transition temperature these coefficients satisfy:

$$\begin{aligned} a &= a\left[\tilde{U}I_0 - \delta\tilde{t}(I_x - I_y)\right] + b\left[\tilde{U}(I_x - I_y) + \delta\tilde{t}(I_{xx} - 2I_{xy} + I_{yy})\right] \\ b &= a\delta\tilde{t}I_0 - b\delta\tilde{t}(I_x - I_y) \end{aligned} \tag{10}$$

where:

$$I_0 = \int_{k_x k_y}^{\epsilon_{k_x k_y}<\epsilon_F} \frac{n(\epsilon_{k_x k_y}/T)}{\epsilon_{k_x k_y}-\epsilon_F}$$
$$I_x = \int_{k_x k_y}^{\epsilon_{k_x k_y}<\epsilon_F} \frac{\cos(k_x) n(\epsilon_{k_x k_y}/T)}{\epsilon_{k_x k_y}-\epsilon_F}$$
$$I_{xx} = \int_{k_x k_y}^{\epsilon_{k_x k_y}<\epsilon_F} \frac{\cos^2(k_x) n(\epsilon_{k_x k_y}/T)}{\epsilon_{k_x k_y}-\epsilon_F} \quad (11)$$

and similar expressions for I_y, I_{xy} and I_{yy}. The function $n(\omega/T)$ is the Fermi-Dirac distribution, and ϵ_F is the Fermi energy.

From eqs.(10), the critical temperature is given by:

$$0 = 1 + \tilde{U} I_0 - 2\delta\tilde{t}(I_x - I_y) + \delta\tilde{t}^2 \left[(I_x - I_y)^2 - I_0(I_{xx} - 2I_{xy} + I_{yy})\right] \quad (12)$$

The integrals in eqs.(11) diverge as $-\log[(N(\epsilon_F)T]$ at low temperatures, where $N(\epsilon_F) \sim \tilde{t}^{-1}$ is the density of states at the Fermi level, and $\tilde{t} = (\tilde{t}_+ = \tilde{t}_-)/2$. As we are assumming a weak orthorhombic distortion, $I_x \approx I_y$. Hence, eq.(12) always has a solution at low temperatures. The critical temperature is given, approximately, by:

$$T_c \sim c_1 \tilde{t} e^{-(c_2\tilde{U})/N(\epsilon_F)\delta\tilde{t}^2} \sim c_1' t e^{-(c_2\Delta^4)/[t^2 N(\epsilon_F) V_{CF}^2 U]} \quad (13)$$

where we assume $t_{dd} \sim t_{sd} \sim t$. c_1 and c_2 are numerical constants. The expression in eq.(13) implies that the superconductivity is supressed as $\Delta \to \infty$. It is enhanced by the the lattice asymmetry, described by V_{CF}, and by the existence of a finite U, as the assisted hopping term requires the presence of electron-electron interactions. Near half filling, the van Hove singularity in the density of states implies $T_c \propto t e^{-c\sqrt{\lambda}}$, where $\lambda = \Delta^4/(tV_{CF}^2 U)$[14,15,16]. The expression in eq.(13) ceases to be valid near the band edges, as $I_{xx} - 2I_{xy} + I_{yy} \to 0$. It can be shown that, in this limit:

$$\lim_{n\to 0} I_{xx} - 2I_{xy} + I_{yy} \propto n \quad (14)$$

where n is the number of carriers per unit cell. Then:

$$\lim_{n\to 0} T_c \sim c_1' t e^{-(c_2\Delta^4)/[ntV_{CF}^2 U]} \to 0 \quad (15)$$

We can also calculate:

$$\frac{a}{b} \sim \frac{\delta\tilde{t}^3 N^2(\epsilon_F)}{U I_0} \sim \frac{t^3 N^2(\epsilon_F) U^2 V_{CF}^3}{\Delta^6} \quad (16)$$

so that $a/b \to 0$ as Δ becomes the largest energy in the problem. In this limit, the gap, eq.(9), will have $d_{x^2-y^2}$ symmetry.

It is interesting to compare the value in eq.(13) with the critical temperature deduced from the Kohn-Luttinger analysis for the Hubbard model without assisted hopping terms, T_{cKL}. The effective coupling constant arises from the screened interaction, and, to lowest order in U, it goes as $U^2 N(\epsilon_F)$. Hence, $T_{cKL} \sim d_1 t e^{-d_2/(UN(\epsilon_F))^2}$. Thus, within the perturbative approach used here, we find $T_c \gg T_{cKL}$, although T_c also depends on the strength of the orthorhombic distortion.

Phase diagram. So far, we have only considered the superconducting instability. Near half filling, it is well known that the hamiltonian in eq.(1) has nesting properties, and antiferromagnetism is favored. The corresponding Nèel temperature is proportional to the gap, so that[17]:

$$T_N \sim b_1 t e^{-b_2/\sqrt{UN(\epsilon_F)}} \quad (17)$$

Assuming that $V_{CF} \ll \Delta$, we find that, near half filling, $T_c \ll T_N$, and the system will be antiferromagnetic. This phase dissappears at densities, measured from half filling, $n \sim e^{-b_2/\sqrt{UN(\epsilon_F)}}$. A sketch of the expected phase diagram is shown in Fig.[2]. Th method used here cannot be used to elucidate the nature of the transition from the antiferromagnetic phase at half filling to the superconducting phase. Hartree-Fock studies of the Hubbard model suggest that an orthorhombic distortion favors the formation of stripes[13]. Alternatively, phase separation is also possible[18]. Higher order terms in $V_{CF}/\Delta, U/\Delta$, not considered here, will break the electron-hole symmetry shown in Fig.[2][10,11]. It is interesting to note that the single band Hubbard model can show an intrinsic tendency towards an orthorhombic distortion near half filling[19].

Conclusions. We have studied a variation of the assisted hopping model, which includes the effects of other atomic levels in Hubbard hamiltonians[10,11] (see also[20]). We have avoided the difficulties associated to intermediate coupling situations by restricting the study to a well defined weak coupling case, where standard perturbation theory is reliable (for a similar approach to other assisted hopping problem, see[21]).

The induced assisted hopping terms lead to d-wave superconductivity. The arguments used here show that the symmetry of the order parameter, for models with different atomic orbitals, is associated to the relative symmetry of these orbitals. When the most relevant orbitals are of the same symmetry, only s-wave superconductivity is possible, in agreement with[10,11]. It is interesting to note that the symmetry of the order parameter does not arise from the anisotropies of the Fermi surface, as for the Kohn-Luttinger mechanism. We have shown, that in the

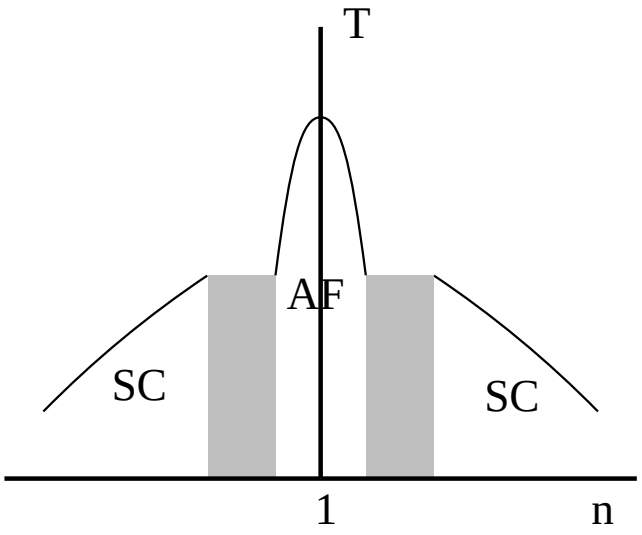

FIG. 2: Sketch of expected phase diagram for the model described by eq.(1), see text for details. The present analysis is insufficient to characterize the intermediate regions between the antiferromagnetic and superconducting phases, shown shaded in the figure.

weak coupling regime, the value of the critical temperature arising from the assisted hopping term tends to be larger than that due to the Kohn-Luttinger mechanism. It is plausible that, in the same manner, the presence of assisted hopping terms will enhance the tendency of the standard Hubbard model towards superconductivity in the intermediate coupling regime.

Finally, the present results can be extended to other systems where assisted hopping terms are likely to arise. In quantum dots, where the sign of these terms can be random[21], they can enhance the tendency towards local pairing.

Acknowledgements. I am grateful to J. E. Hirsch, for sharing his insights in the nature of assisted hopping effects, and for many other helpful discussions. The hospitality of the Kavli Institute for Theoretical Physics, where this work was done, is gratefully acknowledged. The KITP is supported by NSF through grant PHY99-07949. Additional funding comes from MCyT (Spain) through grant PB96-0875.

[1] W. Kohn, and J. M. Luttinger, Phys. Rev. Lett. **15**, 524 (1965).
[2] A. V. Chubukov, and J. P. Lu, Phys. Rev. B **46**, 11163 (1992).
[3] J. González, F. Guinea, and M. A. H. Vozmediano, Europhys. Lett., **34**, 711 (1996). *ibid*, Phys. Rev. Lett., **79**, 3514 (1997).
[4] R. Hlubina, Phys. Rev. B **59**, 9600 (1999). J. Mráz, and R. Hlubina, cond-mat/0212217.
[5] D. J. Scalapino, Phys. Rep. **250**, 329 (1995).
[6] S. R. White, and D. J. Scalapino, Phys. Rev. B **60**, R753 (1999).
[7] M. Calandra, and S. Sorella, Phys. Rev. B **61**, R11894 (2000).
[8] A. I. Lichtenstein, and M. I. Katselson, Phys. Rev. B **62**, R9283 (2000).
[9] Th. Maier, M. Jarrell, Th. Pruschke, and J. Keller, Phys. Rev. Lett. **85**, 1524 (2000).
[10] J. E. Hirsch, and F. Marsiglio, Phys. Rev. B **39**, 11515 (1989).
[11] J. E. Hirsch, Phys. Rev. B **48**, 3327 (1993).
[12] L. Arrachea, A. A. Aligia, E. Gagliano, K. Hallberg, and C. Balseiro, Phys. Rev. B **50**, 16044 (1994).
[13] B. Normand, and A. Kampf, Phys. Rev. B **64**, 024521 (2001).
[14] J. E. Hirsch, and D. J. Scalapino, Phys. Rev. Lett. **56**, 2732 (1986).
[15] J. Labbé, and J. Bok, Europhys. Lett. 3, 1225 (1987).
[16] J. Friedel, J. Phys. (Paris) **48**, 1787 (1987).
[17] J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).
[18] F. Guinea, G. Gómez-Santos, and D. P. Arovas, Phys. Rev. B **62**, 391 (2000).
[19] C. J. Halboth, and W. Metzner, Phys. Rev. Lett. **85**, 5162 (2000).
[20] The Hubbard hamiltonian alone can lead to the low energy effective hamiltonians with assisted, hopping terms, see E. Louis, F. Guinea, M. P. López-Sancho, and J. A. Vergés, Phys. Rev. B **59**, 14005 (1999).
[21] F. Guinea, cond-mat/0212080.